

Ferromagnetic transition in a double-exchange model

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We calculate the temperature of a ferromagnetic transition in a double-exchange model with classical core spins for arbitrary relation between Hund exchange coupling and electron band width by solving the Dynamical Mean Field Approximation equations.

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I. INTRODUCTION

The double-exchange (DE) model [1,2,3] is one of the basic ones in the theory of magnetism. Magnetic ordering appears in this model due to Hund exchange coupling between the core spins and the mobile carriers. The Hamiltonian of the model is

$$H = \sum_{nn'\alpha} t_{n-n'} c_{n\alpha}^\dagger c_{n'\alpha} - J \sum_{n\alpha\beta} \mathbf{S}_n \cdot \sigma_{\alpha\beta} c_{n\alpha}^\dagger c_{n\beta}, \quad (1)$$

where c and c^\dagger are the electrons annihilation and creation operators, \mathbf{S}_n is the operator of core spin, $t_{n-n'}$ is the electron hopping, J is Hund exchange coupling between a core spin and a conduction electron, σ is the vector of the Pauli matrices, and α, β are spin indices.

The model (the core spins being treated as classical vectors) was thoroughly studied already in the papers [1,2,3]. During the last years, because of a general interest in manganites, the model was brought in the focus of attention, and a lot more was achieved (see reviews [4,5,6] and references therein). However, some basic properties of the model are still known only partially. For example, most of the papers dealing with the DE model, starting from classical paper by De Gennes [3], considered the DE Hamiltonian with infinite exchange (and with the addition of the antiferromagnetic superexchange, which is crucial for the explanation of magnetic properties of manganites).

The other extremity which was studied is the particular case of weak exchange (much less than the electron bandwidth), when the DE Hamiltonian can be reduced to Ruderman-Kittel-Kasuya-Yosida (RKKY) Hamiltonian (see review [7] and references therein).

In this paper we calculate the temperature of a ferromagnet - paramagnet transition T_c in a double-exchange model for arbitrary relation between Hund exchange coupling and electron band width by solving the Dynamical Mean Field Approximation equations. Note that we treat the core spins as classical vectors. (When the quantum nature of the core spins is taken into account, the

Hamiltonian (1), which in this case is often called the periodic Kondo model, becomes much more complicated; only scanty results were obtained for the model up to now.) The problem of classical spins, as we shall see, combines tractability with rich and interesting physics.

II. HAMILTONIAN AND DMFA EQUATIONS

Like it was said above, we consider spins as classical vectors $\mathbf{S}_n = \mathbf{m}_n$ with the normalization $|\mathbf{m}|^2 = 1$. Thus the DE Hamiltonian in a single electron representation can be presented as

$$H_{nn'} = t_{n-n'} - J \mathbf{m}_n \cdot \sigma \delta_{nn'}. \quad (2)$$

We have a problem of electron scattered by core spins, the probability of any given core spin configuration depending upon the energy of electron subsystem. To solve the problem we will use the Dynamical Mean Field Approximation (DMFA) (see [8,9] and references therein).

In this approach, first we calculate an averaged, with respect to random orientation of core spins, density of states of electron in a random core spins configuration, treating electron scattering in a single site approximation, and considering the probability of any configuration as given. We introduce Green's function

$$\hat{G}(E) = (E - H)^{-1}, \quad (3)$$

In this approximation the averaged locator

$$\hat{G}_{\text{loc}}(E) = \langle \hat{G}_{nn}(E) \rangle, \quad (4)$$

is expressed through the the local self-energy $\hat{\Sigma}$ by the equation

$$\hat{G}_{\text{loc}}(E) = g_0 (E - \hat{\Sigma}(E)), \quad (5)$$

where

$$g_0(E) = \frac{1}{N} \sum_{\mathbf{k}} (E - t_{\mathbf{k}})^{-1} \quad (6)$$

is the bare (in the absence of the exchange interaction) locator. The self-energy satisfies equation

$$\hat{G}_{\text{loc}}(E) = \left\langle \frac{1}{\hat{G}_{\text{loc}}^{-1}(E) + \hat{\Sigma}(E) + J\mathbf{m} \cdot \hat{\sigma}} \right\rangle, \quad (7)$$

where $\langle X(\mathbf{m}) \rangle \equiv \int X(\mathbf{m})P(\mathbf{m})$, and $P(\mathbf{m})$ is a probability of a given spin orientation (one-site probability). The quantities \hat{G} and $\hat{\Sigma}$ are 2×2 matrices in spin space.

In PM phase $P(\mathbf{m}) = \text{const}$, the averaging in Eq. (7) can be performed explicitly, $\hat{\Sigma} = \Sigma\hat{1}$, $\hat{G} = g\hat{1} = g_0(E - \Sigma)\hat{1}$, where $\hat{1}$ is a unity matrix, and we obtain

$$g(E) = \frac{1}{2} \sum_{(\pm)} \frac{1}{g^{-1}(E) + \Sigma(E) \pm J}. \quad (8)$$

To first approximation of the DMFA, leading to Eq. (7), has a simple physical meaning. We reduce the problem of electron scattering due to many spins, each with the scattering potential $-J\mathbf{m} \cdot \sigma$, to a problem of a scattering due to a single spin with the effective scattering potential $-J\mathbf{m} \cdot \sigma - \hat{\Sigma}$, embedded in an effective medium, described by the Hamiltonian $t_{\mathbf{k}} + \hat{\Sigma}$, and, hence, by locator \hat{G}_{loc} .

The same MF approach leads to the second DMFA approximation - the approximation for the one-site probability $P(\mathbf{m})$, which allows to perform averaging in FM phase. Consider again a single spin with the effective scattering potential in an effective medium. The change in the number of states of the electron gas due to such spin is [10,11]

$$\Delta N(E, \mathbf{m}) = -\frac{1}{\pi} \text{Im} \ln \det \left[1 + \left(J\mathbf{m}\hat{\sigma} + \hat{\Sigma}_+ \right) \hat{G}_{\text{loc}+} \right], \quad (9)$$

where $Y_+ \equiv Y(E + i0)$. So the change in thermodynamic potential is [12,13,14]

$$\beta \Delta \Omega(\mathbf{m}) = \int f(E) \Delta N(E, \mathbf{m}) dE, \quad (10)$$

where $f(E)$ is the Fermi function, the chemical potential is found from the equation

$$n = -\frac{2}{\pi} \int_{-\infty}^{\infty} f(E) \text{Im} g_+ dE, \quad (11)$$

and n is the number of electrons per site. The result for the one-site probability reads:

$$P(\mathbf{m}) \propto \exp[-\beta \Delta \Omega(\mathbf{m})]. \quad (12)$$

Eqs. (7) and (12) are the system of two non-linear (integral) equations for $\hat{\Sigma}(E)$ and $P(\mathbf{m})$, which one should solve to find thermodynamic properties of the model. However, in linear approximation with respect to macroscopic magnetization \mathbf{M} , we can reduce this complicated system to a traditional MF equation for \mathbf{M} [15]:

$$P(\mathbf{m}) \propto \exp(-3\beta T_c \mathbf{M} \cdot \mathbf{m}). \quad (13)$$

The parameter T_c is formally introduced as a coefficient in the linear term of the expansion of $\Delta \Omega(\mathbf{m})$ with respect to \mathbf{M} (the reason for the notation we have chosen and for the numerical coefficient 3 will be clear immediately); it is determined by the properties of the system in paramagnetic phase. Non-trivial solution of the MF equation

$$\mathbf{M} = \langle \mathbf{m} \rangle \quad (14)$$

can exist only for $T < T_c$, hence T_c the Curie temperature.

III. T_c FOR SEMI-CIRCULAR DOS

For simplicity consider the semi-circular (SC) bare density of states (DOS) $N_0(\varepsilon)$, the bandwidth being $2W$. Then

$$g_0(E) = \int \frac{N_0(\varepsilon)d\varepsilon}{E - \varepsilon} = \frac{2}{W} \left[\frac{E}{W} - \sqrt{\left(\frac{E}{W}\right)^2 - 1} \right]. \quad (15)$$

For this case

$$\hat{\Sigma}(E) = E - 2w\hat{G}_{\text{loc}} - \hat{G}_{\text{loc}}^{-1}, \quad (16)$$

where $w = W^2/8$, and Eq. (7) and (8) take respectively the form

$$\hat{G}_{\text{loc}}(E) = \left\langle \frac{1}{E - 2w\hat{G}_{\text{loc}}(E) + J\mathbf{m} \cdot \hat{\sigma}} \right\rangle \quad (17)$$

$$g(E) = \frac{1}{2} \sum_{(\pm)} \frac{1}{E - 2wg(E) \pm J}. \quad (18)$$

Expanding Eq. (17) and then Eq. (9) with respect to \mathbf{M} , after straightforward algebra, for the T_c we obtain

$$T_c = \frac{4J^2w}{3\pi} \int_{-\infty}^{\infty} f(E) \text{Im} \left[\frac{g_+^2}{(E_+ - 2wg_+)(E_+ - 4wg_+) - \frac{4J^2w}{3}g_+^2} \right] dE. \quad (19)$$

Formally speaking because the integral in Eq. (19) contains Fermi function critical temperature enters also into the r.h.s. of the equation. But in all cases T_c turns out to be much less the chemical potential, so we can consider electron gas as degenerate, and Eq. (19) is an explicit formula for calculation of T_c .

Eq. (19) is the main result of our paper. The analysis of this equation let us start from the limiting case $J = \infty$. In this case integral can be calculated explicitly and we obtain [14]

$$T_c = \frac{W\sqrt{2}}{4\pi} \left[\sqrt{1-y^2} - \frac{1}{\sqrt{3}} \tan^{-1} \sqrt{3(1-y^2)} \right], \quad (20)$$

where y is an implicit function of concentration, given by equation $n = \frac{1}{2} - \frac{1}{\pi} \left(\sin^{-1} y + y\sqrt{1-y^2} \right)$. The result coincides with that known previously [9].

For arbitrary exchange the integral can be calculated only numerically, but before we present the results of calculations we should state that in part of the $J/W - n$ plane Eq. (19) gives $T_c < 0$. In fact, like in any MF theory of a second order phase transition, in our calculation of the critical temperature we started from a high temperature paramagnetic phase and decreasing the temperature were looking for an instability of a model with respect to appearance of small spontaneous magnetic moment that is for the appearance of a nontrivial solution of the MF equation. Negative T_c in some part of the $J/W - n$ plane means, that at any temperature, including $T = 0$, the paramagnetic phase here is stable with respect to the appearance of small spontaneous magnetic moment even at $T = 0$, and excludes ferromagnetism in that region of the plane. The part of the critical surface corresponding to the region of the parameters plane where $T_c \geq 0$ is presented on FIG. 1.

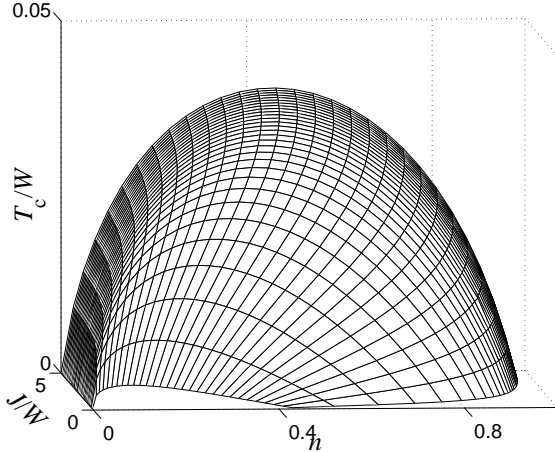


FIG. 1. T_c as a function of relative strength of the Hund exchange J/W and electron concentration n .

IV. DISCUSSION

Let us finally discuss, whether the PM-FM transition observed with decreasing temperature can be preceded by the transition from the the PM phase to some magnetic phase other than FM (say, antiferromagnetic)? We would like to present some heuristic arguments that this is not the case.

First, consider the case of weak exchange $J \ll W$. In this case Eq. (19) takes the form

$$T_c = \frac{2J^2}{3} \int_{-\infty}^{\infty} f(E) \left\{ \frac{dN_0(E)}{dE} - \frac{1}{\pi} \text{Im } g_0(E_+)^2 \right\} dE. \quad (21)$$

In fact, this equation is the MF approximation [15] for the RKKY Hamiltonian [7], to which the original Hamiltonian (1) can be reduced to in the case $J \ll W$. So Eq. (21) does not involve either the coherent potential approximation (Eq. (7)), or the SC density of states.

Anyhow, for the SC density of states we use, Eq. (21) gives ferromagnetic ground state for $n < 0.4$, which qualitatively agrees with the result of numerical calculations, giving FM ground state for $n < 0.25$ for the three principal cubic lattices [16].

To formulate the second argument, let us compare the energies of the PM state

$$E_p = -\frac{2}{\pi} \int_{-\infty}^{E_F^{(p)}} E \text{Im } g_+ dE; \quad (22)$$

and of the saturated FM state

$$E_f = \int_{-\infty}^{E_F^{(f)}} E \sum_{(\pm)} N_0(E \pm J) dE, \quad (23)$$

where E_F is the appropriate Fermi energy. On fig. 2 we plotted simultaneously the curve given by by equation $E_p = E_f$ and by equation $T_c = 0$, where T_c is obtained from Eq. (19).

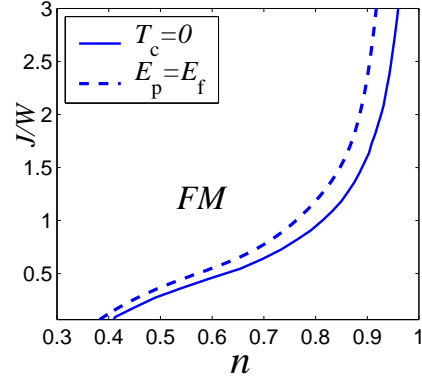


FIG. 2. The FM region boundary in the coordinates of relative strength of the Hund exchange J/W and electron concentration n .

The close vicinity of the abovementioned curves supports the belief that the curve $T_c = 0$ is the quantum critical line (see [17] and references therein), which bounds *ferromagnetic* phase. Also, the boundary of ferromagnetic phase on FIG. 2 agrees with those obtained on the basis of numerical calculations [18] and from qualitative reasoning [13].

The destruction of ferromagnetic ground state occurs because finite double exchange between the itinerant electrons and core spins, unlike an infinite one, by itself generates effective antiferromagnetic exchange between the core spins (which was absent in original Hamiltonian).

Due to the fact that our main result (equation for the transition temperature) indicates its own limits of validity, we can find the boundaries of ferromagnetic phase without analyzing what phases are beyond the boundaries.

Finally, we would like to mention, that in the DMFA, as one can easily see from Eq. (7), density of electron states in paramagnetic phase does not depend upon electron concentration. In this case, the derivative of chemical potential with respect to number of electrons is just the inverse density of states at the Fermi level (for the degenerate electron gas), and is always positive. Hence, there is no phase separation in paramagnetic phase.

In conclusion, we explicitly formulated the Dynamical Mean Field Approximation equations for the double exchange model with classical spins for arbitrary relation between Hund exchange and the electron bandwidth. Near paramagnetic-ferromagnetic transition critical point, these equations were reduced to a MF equation, describing a single spin in an effective field, proportional to the macroscopic magnetization. The effective exchange interaction, entering into the MF equation was found for the semicircular electron density of states. We thus calculated the transition temperature T_c as a function of Hund exchange interaction and electron density in the whole parameters plane. The results obtained also allow to plot the boundaries of the ferromagnetic region on the model phase diagram.

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